

Role of Inelastic Tunneling through the Barrier in Scanning Tunneling Microscope Experiments on Cuprates

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The tunneling path between the CuO_2 -layers in cuprate superconductors and a scanning tunneling microscope tip passes through a barrier made from other oxide layers. This opens up the possibility that inelastic processes in the barrier contribute to the tunneling spectra. Such processes cause one or possibly more peaks in the second derivative current-voltage spectra displaced by phonon energies from the density of states singularity associated with superconductivity. Calculations of inelastic processes generated by apical O-phonons show good qualitative agreement with recent experiments reported by Lee et al. [1]. Further tests to discriminate between these inelastic processes and coupling to planar phonons are proposed.

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The importance of the electron-phonon interaction in the high temperature cuprate superconductors has long been a matter of debate. In conventional superconductors tunneling experiments analyzed by McMillan and Rowell [2] not only unequivocally established that the exchange of phonons between electrons is the underlying mechanism for Cooper pairing but also allowed its spectroscopic determination. In the case of cuprates there are many good reasons to doubt the dominance of an attraction due to phonon exchange. These reasons range from the d-wave rather than s-wave pairing symmetry, to their electronic structure as lightly doped Mott insulators. The latter points toward a strong onsite Coulomb repulsion which cannot be treated perturbatively, violating a key postulate in the standard BCS-Eliashberg theory. A number of proposals have been made for a subdominant role for the electron-phonon interactions particularly involving the half-buckling phonon modes which couple attractively in the d-wave pairing channel [3, 4, 5, 6, 7, 8].

Very recently, a new set of tunneling measurements at low temperatures has been reported by Lee et al. [1] using a STM (Scanning Tunneling Microscope). Results with this local tunneling probe show considerable variations in the form and energy of the density of states (DOS) singularity associated with the superconductivity and also a peak in the second derivative current-voltage spectra which is displaced from the DOS peak by a fairly constant energy. Lee et al. [1] report further that isotope substitution on the O-ions shifts this energy consistent with a phonon origin for this peak. This raises the question whether these spectra should be interpreted analogously to those of conventional superconductors or if these peaks have another source.

A series of works explain the appearance of side peaks in the DOS of d-wave superconductors in terms of localized bosonic modes [9], resonant spin modes [10, 11] or the breathing mode phonons [12]. All these proposals consider inelastic processes that happen directly in

the superconducting plane. In this letter we examine an alternative explanation in terms of inelastic tunneling processes. Such inelastic processes are well established in electron tunneling spectroscopy [13, 14, 15, 16] of metal-insulator-metal junctions and in STM spectra taken on metals with adsorbed molecules [17, 18]. In cleaved BSSCO the topmost layer is the BiO-plane, but the electrons tunnel into and out of the CuO_2 -planes. Inelastic tunneling can occur in the intervening barrier, e.g. when the tunneling hole passes through the apical O-ion. Although the $2p_z$ -orbitals of the apical O-ion do not hybridize with the $3d_{x^2-y^2}$ -orbitals of the Cu-ion directly below there is a weaker hybridization with orbitals centered on neighboring Cu-ions [19]. However we will not go into such details here. Rather, we examine a simple model which has an important tunneling path through an apical O-orbital removed from the chemical potential.

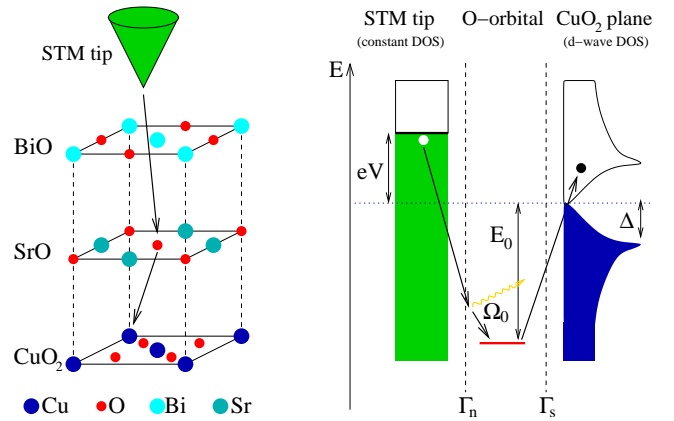


FIG. 1: **Left panel:** Geometry relevant for the scanning tunneling microscope experiment, the superconducting CuO_2 -plane lies below BiO- and SrO-layers. **Right panel:** Suggested inelastic cotunneling process via the apical oxygen atom leading to phonon-satellites in the current-voltage characteristics in electron-energy scheme.

This tunneling path is in turn coupled to a vibration of this ion. Our aim is to establish the key features of this inelastic tunneling process and to compare them to the experimental spectra.

Our aim is to calculate the cotunneling current through the $2p_z$ -orbital of the apical O-ion. For this purpose we describe the setup depicted in Fig. 1 by the Hamiltonian,

$$H = H_n + H_s + H_t$$

$$+ E_0 \sum_s p_s^\dagger p_s + \sum_q \omega_q b_q^\dagger b_q + \sum_{qs} M_q p_s^\dagger p_s (b_q + b_{-q}^\dagger), \quad (1)$$

where H_n represents the normal conducting STM tip, H_s the superconducting CuO_2 -plane and H_t the hopping onto the apical oxygen orbital. Operator p_s^\dagger creates a hole in the oxygen p-orbital, operator b_q^\dagger creates a phonon with momentum q . The STM tip is characterized by a constant DOS $N_n(\varepsilon) \propto n_n(\varepsilon) = 1$. Partial line widths Γ_n, Γ_s of the $2p_z$ -orbital at energy E_0 are used to describe its hybridization with the STM tip and the superconducting CuO_2 -plane. As we shall discuss at the end of this section the above parameters mainly affect the overall prefactor in the tunneling current and are not very crucial. The shape of the current-voltage characteristics is determined by the DOS of the superconductor and the phonon spectrum. For the superconductor we assume for simplicity a d-wave type DOS $N_s(\varepsilon) \propto n_s(\varepsilon) = \langle \text{Re} [\varepsilon / \sqrt{\varepsilon^2 - \Delta^2 \cos^2 \theta}] \rangle_\theta$. However, in the experiment [1] the shape of the superconducting DOS varies strongly from point to point. Since the phonon involves mainly the motion of the apical oxygen atoms we assume an optical phonon band centered around frequency Ω_0 with a weak dispersion (i.e. a small band width W).

The derivation of the cotunneling current follows closely Ref. [20] which deals with a similar non-equilibrium situation in the normal conducting state. Tunneling is treated to lowest order, while electron-phonon coupling is treated non-perturbatively allowing for multi-phonon processes. Applying a Lang-Firsov transformation [21] and standard manipulations of many-body physics [22] one arrives at the following expression for the cotunneling current (we set $\hbar = 1$)

$$I(V) = \frac{e\Gamma_n\Gamma_s}{2\pi} \int \frac{F_n(\varepsilon)\bar{F}_s(\varepsilon) - F_s(\varepsilon)\bar{F}_n(\varepsilon)}{(\varepsilon - E_0)^2 + |\Sigma(\varepsilon)|^2} d\varepsilon. \quad (2)$$

The factors $F_x(\varepsilon), \bar{F}_x(\varepsilon)$ with $x = n, s$ are obtained from a convolution,

$$\begin{pmatrix} F_x(\varepsilon) \\ \bar{F}_x(\varepsilon) \end{pmatrix} = \int d\omega n_x(\varepsilon + \omega) \begin{pmatrix} B(\omega) f_x(\varepsilon + \omega) \\ B(-\omega) [1 - f_x(\varepsilon + \omega)] \end{pmatrix}, \quad (3)$$

of the relevant DOS, $n_x(\varepsilon)$, and the Fermi factors, $f_x(\varepsilon)$, with the phonon correlation function $B(\omega)$. The lat-

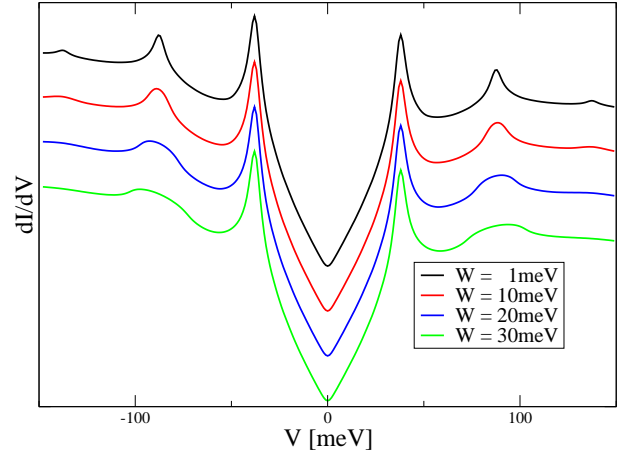


FIG. 2: Shape of dI/dV for different widths W of the phonon band. Parameters are $\Delta = 38\text{meV}$, $\Omega_0 = 50\text{meV}$, $\lambda = 0.4$, $E_0 = 2\text{eV}$.

ter will be discussed in detail below. The retarded self-energy $\Sigma(\varepsilon)$ of the $2p_z$ -orbital reads

$$\Sigma(\varepsilon) = -\frac{i}{2} \sum_{x=n,s} \Gamma_x \{F_x(\varepsilon) + \bar{F}_x(\varepsilon)\}. \quad (4)$$

If the energy E_0 of the virtual oxygen state is the largest energy scale in the problem, the energy dependence of the denominator of Eq. (2) can be neglected [23]. In this case, we may approximate the tunneling current by

$$I(V) \sim \int \{F_n(\varepsilon)\bar{F}_s(\varepsilon) - F_s(\varepsilon)\bar{F}_n(\varepsilon)\} d\varepsilon \quad (5)$$

and the parameters E_0, Γ_n, Γ_s describing the virtual state enter only in the (unimportant) prefactor. Even if terms with $\varepsilon \simeq E_0$ contribute significantly to the integral (2), the energy dependence of the denominator will only lead to an asymmetry of the current-voltage signal on a larger energy scale. In the following, we therefore concentrate on the influence of the phonon spectrum which creates the sharp features visible in the experiment [1].

The phonon spectrum enters the current-voltage spectrum (2) via the modified occupation factors (3). In Eq. (3), the phonon correlation function $B(\omega) = (2\pi)^{-1} \int dt e^{i\omega t} \langle X(t) X^\dagger(0) \rangle$ describes possible phonon emission or absorption of the oxygen $2p_z$ -orbital. Those processes lead to an effective shift of the Fermi occupation factors of both the superconducting plane and the normal conducting STM tip. The “displacement” operator $X = \exp \left\{ \sum_q M_q (b_q - b_{-q}^\dagger) / \omega_q \right\}$ results from a Lang-Firsov transformation [21]. Replacing the q -summation by a frequency integration over a box density of states and assuming zero temperature for the phonon bath we obtain the correlation function

$$\langle X(t) X^\dagger(0) \rangle = \exp \left\{ \lambda^2 \left(\frac{2}{Wt} \sin \frac{Wt}{2} e^{-i\Omega_0 t} - 1 \right) \right\} \quad (6)$$

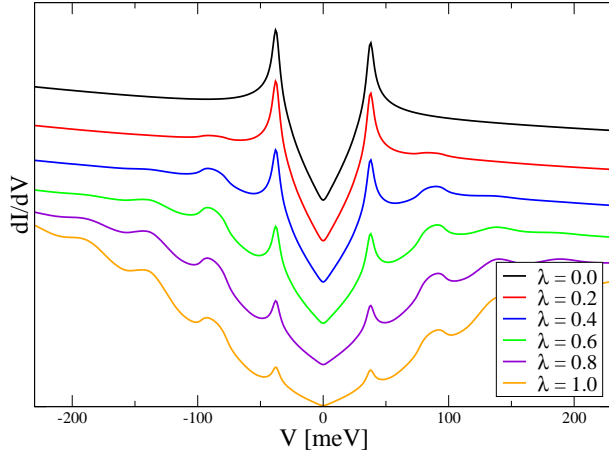


FIG. 3: Shape of dI/dV for different electron-phonon couplings λ . Parameters are $\Delta = 38\text{meV}$, $\Omega_0 = 50\text{meV}$, $W = 20\text{meV}$, $E_0 = 2\text{eV}$.

which is used in the following numerical calculations. The parameter λ measures the strength of electron-phonon coupling, Ω_0 is the mean phonon frequency, W defines the band width. Note that this correlation function takes into account multiple phonon emissions. A purely perturbative treatment corresponds to the expansion of the exponential in Eq. (6) to quadratic order in the coupling constant λ .

Fig. 2 shows the differential tunneling conductance dI/dV for different widths of the optical phonon band. The phonon satellites are most clearly visible in the case of completely localized Einstein phonons ($W = 1\text{meV}$). Each satellite then reproduces exactly the singularity of the quasiparticle peak in the superconducting DOS. The case of Einstein phonons seems to be excluded by the experimental data which shows broadened phonon satellites. Comparing qualitatively peak heights and peak widths of theory and experiment, we are led to the conclusion that the phonon band has a width of roughly 20meV . This width is probably due to the vibrational coupling of the apical oxygen atom to its neighbors. Since the electron-phonon coupling constant is quite large one might also expect broadening due to particle-hole excitations in the superconducting plane or due to the anharmonicity of the crystal leading to a finite phonon lifetime.

In Fig. 3 we show the dependence of the differential conductance on the electron-phonon coupling strength λ . The stronger the coupling the more phonon satellites become visible in the spectrum. The amplitude of the n th satellite is smaller than that of the $n - 1$ th satellite by roughly a factor of λ^2/n . A comparison of first and second satellite therefore allows for an estimate of the coupling strength λ . From the experimental data we estimate $\lambda \simeq 0.4$.

Fig. 4 evaluates the isotope effect in the second deriva-

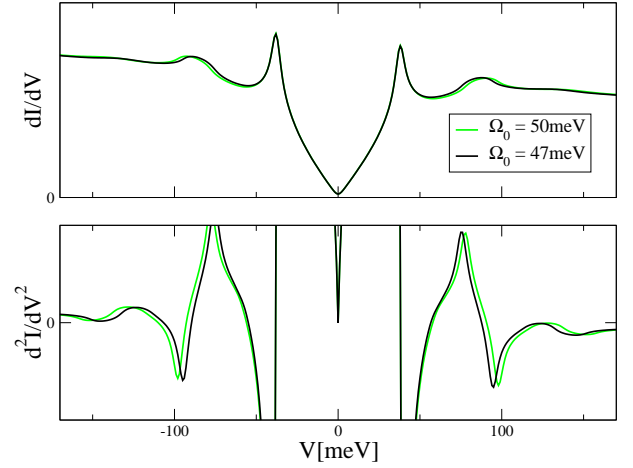


FIG. 4: Isotope shift in the d^2I/dV^2 . Parameters are $\Delta = 38\text{meV}$, $\Omega_0 = 50\text{meV}$, $W = 20\text{meV}$, $\lambda = 0.4$, $E_0 = 2\text{eV}$. The sign in the d^2I/dV^2 for negative voltages has been flipped.

tive d^2I/dV^2 of the current-voltage spectrum as measured in the experiment [1]. The isotope effect is most clearly visible for the first satellite which stems from a single convolution of the quasiparticle peak with the phonon spectrum. The second satellite stems from a twofold convolution with the phonon spectrum. Its second derivative d^2I/dV^2 is therefore much smoother, and the isotope effect less well seen.

Experimentally [1], the lowest phonon frequency is obtained as the energy difference between the quasiparticle peak in the dI/dV (in our case at 38meV) and the maximum of the second derivative d^2I/dV^2 (in our case at 78meV). This procedure is standard in conventional superconductivity where the strong singularity in the s-wave density of states guarantees a pronounced feature in the second derivative d^2I/dV^2 . In the case of d-wave superconductivity this singularity is much weaker and consequently the maxima in the second derivative are less well defined. If the quasiparticle peak is weakened or if the second phonon satellite is investigated another procedure to determine the phonon frequencies can be preferable: Determining the positions of both maximum and minimum in the second derivative and taking their average one can directly estimate the central frequency of the phonon band.

Inelastic tunneling processes show up as a pronounced peak in the d^2I/dV^2 spectrum displaced by a phonon energy from the main peak in the dI/dV associated with the DOS singularity which accompanies d-wave superconductivity. The strength and form of the peak reflects those of the DOS singularity. This feature agrees with experiments of Lee et al. [1]. A weaker signal also appears displaced by twice the phonon energies in agreement with experiment. The phonon energy, 50meV , chosen to agree with the experimental spectra, is close to the value ex-

pected for an apical O-phonon and rather higher than the energy of the B_{1g} half-buckling mode [25]. One point of divergence between the theory and the spectra reported by Lee et al. is the presence of a sharp minimum in the calculated d^2I/dV^2 spectra just above the peak.

The STM experiments of Lee et al. [1] show substantial spatial variations in the spectra with a clear correlation between the frequency shift of the side peaks and the local value of the superconducting energy gap. Such a correlation follows if the local bosonic mode couples directly to the planar holes and if this electron-boson coupling is involved in the superconductivity. In our model, unlike those of Refs. [9, 10, 11, 12], such an explanation does not apply. However it is known empirically that the positions of the apical O-ions influences the transition temperature T_c of BSSCO superconductors [26] and more generally that materials with longer Cu-apical O bonds have higher values of T_c [27]. Therefore the anticorrelation between the local magnitude of the superconducting gap and the local size of the frequency shift may reflect this empirical trend and is not incompatible with our model which ascribes these side peaks to inelastic tunneling processes in the barrier.

Lee et al. [1] report an isotope shift when all O-sites are occupied by O^{16} vs. O^{18} . A selective isotope replacement only on the apical O-sites would discriminate between our proposal that the structure is due to apical O-phonons rather than due to the half-buckling mode involving displacements of planar O-ions.

In summary we conclude that inelastic tunneling processes involving the apical O-ions are a viable explanation of the phononic structure in the STM tunneling spectra recently observed by Lee et al. and we propose selective isotope substitution as a test of our proposal.

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